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SiGe and SiGeC Surface Alloy Formation Using High-dose Implantation and Solid Phase Epitaxy

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Abstract -- SiGe is a promising alloy system for VLSI technology. In this study, surface SiGe and SiGeC alloys were formed using high-dose germanium and carbon implantation and subsequent solid phase epitaxial growth (SPEG). RBS channeling spectra and cross-sectional TEM studies show that high quality SiGe and SiGeC alloys were formed with germanium concentration up to 8 at. %, while extended defects were formed in the alloys with 16 at. % germanium. X-ray diffraction experiments show that carbon reduces the lattice strain in SiGe alloys. However, no significant crystallinity improvement was observed under RBS channeling spectra or XTEM observations. Excessive carbon dose also introduces polycrystalline layer formation. Deep level states were found in carbon implanted wafers using temperature-dependent Hall effect measurements.

I. Introduction

In the last 30 years the rapid advances of silicon integrated circuit technology have mostly been based on scaling down the feature size of individual devices. However, as the scaling reaches deep submicron, limitations physical, technological and economical have emerged [1]. One of the possible methods to sustain the advances of the integrated circuit technology is to find materials with improved properties over silicon. Recent studies demonstrate that SiGe alloys grown on Si have significant potential for the fabrication of high speed devices [2]. SiGe can be used for bandgap engineering and strain engineering in Si based VLSI technology. For bandgap engineering, SiGe heterojunction bipolar transistors (HBT's) have high current gain and superior speed because the heterojunction significantly improves the emitter injection efficiency [2, 3]. Using the bandgap engineering concept, SiGe heterojunction can be used in the source/drain region of MOSFET devices to reduce the contact resistance, and to reduce drain induced barrier lowering (DIBL) effect. SiGe was also reported to retard boron diffusion [4], therefore beneficial for shallow junction when used in the source/drain region. Strain in the SiGe/Si heterojunction can change the band structure, hence the carrier effective mass, and most importantly the carrier mobility. Using the strain engineering concept, SiGe channel field effect transistors (FET's) have been fabricated, which have 4 - 5 times higher carrier mobility and transconductance as compared to equivalent Si devices [5].

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The SiGe material system has been extensively studied by researchers using synthesis techniques such as molecular beam epitaxy (MBE) [3, 6], ultra-high vacuum chemical vapor deposition (UHV-CVD) [7], rapid thermal chemical vapor deposition (RTCVD) [8] and ion implantation with subsequent solid phase epitaxial growth (SPEG) [9-11]. The high-dose germanium implantation process is advantageous over direct epitaxial methods because it is compatible with conventional Si processing technology, and can readily be integrated into a standard IC process sequence. However, crystal defects introduced either by the implantation process, such as the end of range (EOR) dislocation loops, or by strain induced defects must be eliminated for any device applications.

Recently, interest in the group IV SiGe system has extended to the SiGeC ternary system [10, 11]. One of the fundamental difficulties to form defect-free $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ heterojunction is due to the 4% lattice constant mismatch between Si ($a_{\text{Si}} = 0.357 \text{ nm}$) and Ge ($a_{\text{Ge}} = 0.356 \text{ nm}$). C is the only element in group IV with a single crystal (diamond) lattice constant less than Si, and has the potential to compensate the built-in strain in the SiGe system. Recent work by Im et al. [10] has demonstrated that $\text{Si}_{1-x}\text{Ge}_x\text{C}_y$ shows less strain induced dislocation formation than $\text{Si}_{1-x}\text{Ge}_x$ alloy. Being isoelectronic with Si and Ge, C is not expected to be a dopant. Nevertheless, it is also known that C inhibits the kinetics of Si SPEG such that a low growth rate is expected. In this paper, we will present results of forming near surface SiGe and SiGeC alloys using the high-dose implantation technique.

II. SiGe and SiGeC Processing

CZ grown p-type 16-24 ohm-cm, (100) Si wafers were implanted with germanium and/or carbon using either a conventional implanter or a metal-vapor vacuum arc (MEVVA) source [12]. Different from conventional implanters, the MEVVA source provides a high current density implantation using solid Ge and C (graphite) sources. Using a conventional implanter, the Ge^+ ions were implanted at an acceleration voltage of 50 kV with two different doses: $1.8 \times 10^{16} \text{ cm}^{-2}$ and $3.6 \times 10^{16} \text{ cm}^{-2}$ with respective peak germanium concentrations of $4 \times 10^{21} \text{ cm}^{-3}$ and $8 \times 10^{21} \text{ cm}^{-3}$. The corresponding germanium content is 8 at. % and 16 at. % respectively. For some of the Ge^+ implanted wafers, C^+ ions were subsequently implanted at 10 kV with one tenth of the corresponding germanium dose.

This energy was chosen to control carbon projected range to be the same as the germanium. In another series of wafers, germanium ions with a dose of $8.0 \times 10^{15} \text{ cm}^{-2}$ were implanted at 20 kV using the MEVVA source. Both single charged Ge^+ and double charged Ge^{++} were produced by the MEVVA ion source with the composition ratio of 60% and 40% respectively. Without mass/charge selective devices, both Ge^+ and Ge^{++} were implanted at 20 kV simultaneously. The C ions produced in the MEVVA source were single charged C^+ , and a dose of $2.0 \times 10^{15} \text{ cm}^{-2}$ C^+ were implanted at 10 kV following the Ge implantation. In this paper, only sample $\text{Si}_{0.95}\text{Ge}_{0.04}\text{C}_{0.01}$ is implanted using the MEVVA source. After the implantation, passivation layers of 50 nm oxide and 50 nm nitride were coated on the wafer surface using plasma enhanced chemical vapor deposition (PECVD) at 300 °C. These passivated wafers were then furnace annealed at temperatures between 700 °C and 1100 °C for 30 minutes in N_2 ambient.

III. Characterization Results

Secondary ion mass spectrometry (SIMS) measurement was used to find the implanted germanium and carbon profile. As seen in Fig. 1, germanium and carbon were implanted at the same depth, and the ratio between germanium and carbon is about 10:1. The germanium profile was also derived from Rutherford backscattering spectroscopy (RBS) measurement. Results from RBS and SIMS correlate well with each other. Nevertheless, carbon profile and concentration can not be derived from RBS spectrum because the concentration is too small (~1-2%), and the signal is overlapped with that from the background Si.

RBS channeling spectra were used to characterize the crystalline quality of these samples. Fig. 2 shows a series of <111> channeling spectra for sample $\text{Si}_{0.91}\text{Ge}_{0.08}\text{C}_{0.01}$ before and after annealing at different temperatures. As shown in the spectra, the as-implanted sample shows a 80 nm amorphous layer at the surface. After annealed at 700 °C or

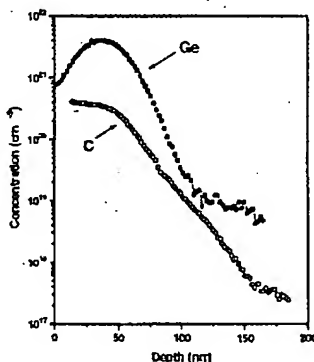


Fig. 1. SIMS profile of as-implanted sample $\text{Si}_{0.91}\text{Ge}_{0.08}\text{C}_{0.01}$ (with 8 at. % germanium and 1 at. % carbon peak concentrations).

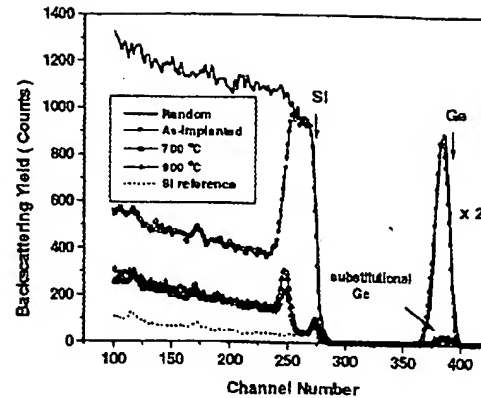


Fig. 2. RBS <111> channeling spectra of $\text{Si}_{0.91}\text{Ge}_{0.08}\text{C}_{0.01}$. The RBS experiments were performed using 2 MeV He^{++} ions at a scattering angle of 165°. The channel resolution was 3.57 kV/Channel.

beyond, the amorphous layers recrystallize into single crystal, revealed by the substitutional germanium signals, and the low channeling yield of Si. The high scattering yield near the original amorphous/crystal interfaces is related to EOR loops. This scattering yield is reduced when the annealing temperature is increased from 700 °C to 900 °C. Little improvement is obtained when the annealing temperature is raised to 1100 °C. EOR defects are formed by the interstitial atoms knocked into crystal during implantation, and it is very difficult to eliminate them after a high dose implantation. A summary of the RBS channeling yield results are presented in Table I. As the germanium peak concentration is at $4 \times 10^{21} \text{ cm}^{-3}$ (8 at. %), channeling yields between 4.3 % and 4.5 % is detected in the alloys. For samples with 16 at. % germanium peak concentration, the channeling yields are between 23% and 27%, significantly higher than that of a defect free Si crystal, indicating extended defects in the alloys. We also notice that in RBS channeling spectra, no significant difference in the crystal quality between samples with or without carbon implantation.

Cross-sectional transmission electron microscopy (XTEM) experiments were conducted to examine defect types and depth distribution of the SPEG layers. XTEM images of sample $\text{Si}_{0.91}\text{Ge}_{0.08}\text{C}_{0.01}$ and $\text{Si}_{0.82}\text{Ge}_{0.16}\text{C}_{0.02}$ are shown in

Table I. Summary of the <111> channeling yields of the alloys
The channeling yield was measured using the integrated germanium χ_{Ge} (Ge), and that from Si near the peak germanium concentration χ_{Si} (Si). The channeling yield from the virgin Si reference wafer is 3.1%.

| | Peak Ge Conc.(at. %) | Peak C Conc.(at. %) | χ_{Ge} (%,Ge) | χ_{Si} (%,Si) |
|---|-------------------------|------------------------|------------------------------|------------------------------|
| $\text{Si}_{0.91}\text{Ge}_{0.08}$ | 8 | 0 | 4.6 | 4.3 |
| $\text{Si}_{0.91}\text{Ge}_{0.08}\text{C}_{0.01}$ | 8 | 0.8 | 4.6 | 4.8 |
| $\text{Si}_{0.84}\text{Ge}_{0.16}$ | 16 | 0 | 27.0 | 26.7 |
| $\text{Si}_{0.82}\text{Ge}_{0.16}\text{C}_{0.02}$ | 16 | 1.6 | 23.6 | 24.2 |

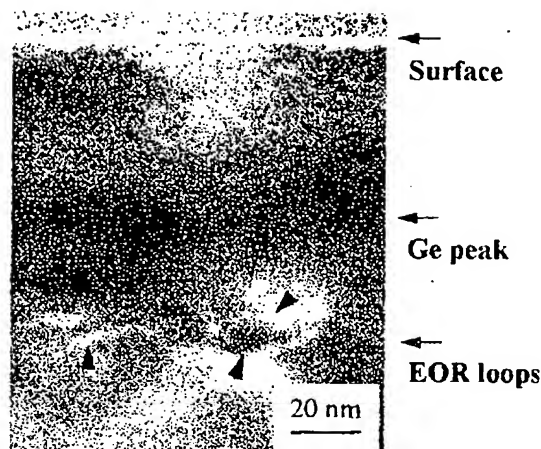


Fig. 3. XTEM micrograph of $\text{Si}_{0.91}\text{Ge}_{0.08}\text{C}_{0.01}$ (SPEG at 900 °C for 30 minutes) shows EOR defects at the original amorphous/crystal interface region.

Fig. 3 and Fig. 4 respectively. For sample $\text{Si}_{0.91}\text{Ge}_{0.08}\text{C}_{0.01}$ shown in Fig. 3, a perfect single crystal is formed at the Ge/C rich region, even though EOR clusters were found at about 80 nm underneath the surface. However for sample $\text{Si}_{0.82}\text{Ge}_{0.16}\text{C}_{0.02}$ shown in Figure 4, extended defects indicated by localized Moiré patterns are visible in the Ge/C rich region. There is no significant difference in the crystal quality between samples with or without carbon implantation from XTEM observation.

Since germanium has a larger lattice constant than Si, we expect compressive strain in the epitaxial alloy layers. The strain was examined using x-ray diffraction method near the Si (004) peak. In the x-ray rocking scan curves shown in Fig. 5, the satellite peak from $\text{Si}_{0.91}\text{Ge}_{0.08}\text{C}_{0.01}$ is much closer

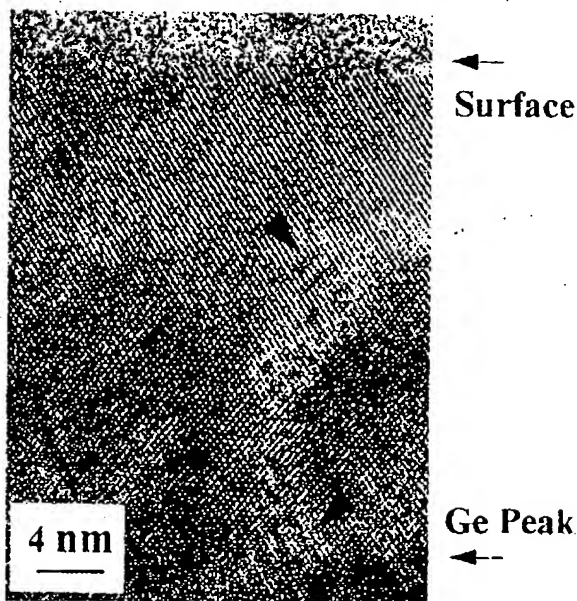


Fig. 4. High resolution XTEM micrograph of $\text{Si}_{0.82}\text{Ge}_{0.16}\text{C}_{0.02}$ (SPEG at 900 °C for 30 minutes) shows localized Moiré patterns pointed by arrow marks. The lattice fringes are from Si (111) planes with a 0.314 nm spacing.

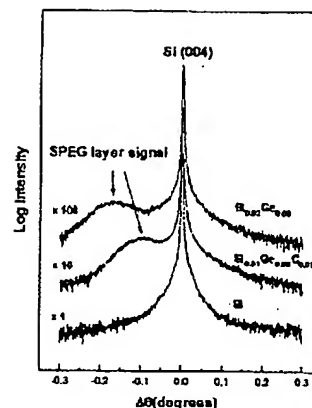


Fig. 5. X-ray rocking curves from $\text{Si}_{0.91}\text{Ge}_{0.08}\text{C}_{0.01}$, $\text{Si}_{0.82}\text{Ge}_{0.16}\text{C}_{0.02}$ and virgin Si near the Si (004) peak. The x-ray rocking scan was performed using a high resolution Siemens D5000 X-ray Diffractometer with a four-bounce Ge crystal monochromator. The x-ray source is $\text{Cu K}\alpha_1$.

to the Si (004) peak than that from $\text{Si}_{0.92}\text{Ge}_{0.08}$, showing a lattice constant closer to Si. This result indicates that carbon incorporation has relieved the strain formation in the SiGe alloys. X-ray diffraction rocking curves near Si (224)₁ and (224)₂ peaks show no lattice expansion in the azimuthal plane at these samples. The lattice constant and the alloy composition can be derived from the satellite diffraction peaks using the pseudomorphic lattice growth mismatch relation [13]. A germanium concentration of 6 at. % is derived. This value agrees with the germanium dose in $\text{Si}_{0.92}\text{Ge}_{0.08}$ (8 at. % peak concentration). The satellite peaks detected from these alloys are quite broad due to the fact that the alloy layer is quite thin (about 80 nm), and there is a depth distribution of the Ge/C concentration.

Due to the high C/Ge ratio, the MEVVA implanted sample $\text{Si}_{0.95}\text{Ge}_{0.04}\text{C}_{0.01}$ shows different SPEG characteristics. Fig. 6 shows the $\langle 111 \rangle$ channeling spectrum of this sample just after implantation (as-implanted), and after annealed at different temperatures for 30 minutes. The original amorphous layer thickness is about 95 nm based on RBS energy loss analysis. The crystal epitaxial growth starts at less than 600 °C (not shown in Fig. 6). However, even at 900 °C, the epitaxial growth stops at about 62 nm, near the Ge and C-rich area. At this temperature, no detectable substitutional Ge is found. At 1000 °C, the epitaxial layer grows further into the Ge and C high concentration area. However, the growth terminates at about 44 nm from the surface. Partial Ge substitution in the epitaxial layer is also found in the Ge channeling profile. The exact physical nature of the alloy structure that causes the strong dechanneling beyond 44 nm can not be determined from the RBS spectrum. Later XTEM results show that the alloy is polycrystalline. At 1100 °C, the epitaxial growth finally reaches the surface as shown in Fig. 6.

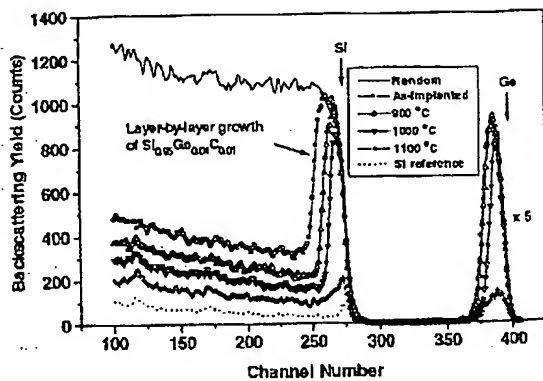


Fig. 6. RBS $\langle 111 \rangle$ channeling spectra of MEVVA implanted sample $\text{Si}_{0.93}\text{Ge}_{0.07}\text{C}_{0.01}$.

Temperature dependent Hall effect measurements were conducted to measure the dopant activation and carrier mobility. Samples were cooled by a liquid-helium cryostat and the temperature variation during each data measurement was less than 0.3°C . In Fig. 7, the linear decrease (in a log plot) of hole concentration at the temperatures less than 100 K is due to the boron doping in the original p-type wafer. However, an abnormal hole concentration increase is found between 200 K and 300 K in the carbon implanted sample. The extrapolated slope of the plot gives a dopant activation energy of about 95 meV, a relatively deep level center. No such effect was found in germanium-only implanted samples.

IV. Conclusions

In summary, SiGe surface alloys were successfully synthesized using high dose germanium implantation into Si, followed by subsequent SPEG. Based on our implantation and annealing sequence experiment, the maximum germanium dose that can be incorporated into Si without forming extended defects is between 8 and 16 at. %. Our experiment showed that carbon reduced the lattice strain in SiGe alloys. Nevertheless, no significant crystal quality improvement was observed by RBS channeling spectra or XTEM observations. Excessive carbon dose can cause polycrystalline formation. Temperature-dependent Hall effect measurement results implicated a formation of deep level centers with the carbon implanted samples.

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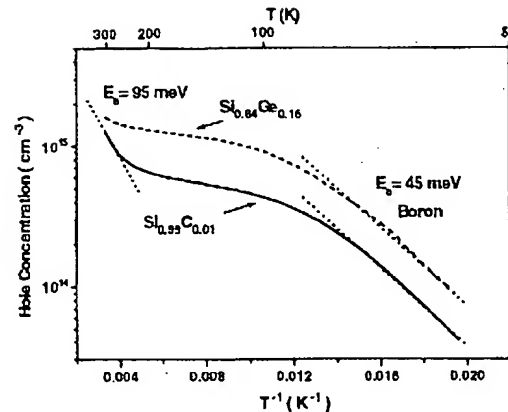


Fig. 7. Temperature dependent Hall hole concentration of sample $\text{Si}_{0.93}\text{C}_{0.01}$ and $\text{Si}_{0.94}\text{Ge}_{0.06}$. $E_a = 45$ meV is the activation energy of Boron. $E_a = 95$ meV is the extracted activation energy from the carbon implanted sample.

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